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by William A. Gordon and Anne K. Gallagher

Lewis Research Center

Cleveland, Ohio

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SUMMARY

Calculations required to convert photographic densities of spectral lines to the concentration-related intensity parameter in spectrographic analysis have been programmed for digital computer processing.

The program produced an emulsion calibration curve for each data set and converted all percent transmission values to relative intensities. Further, the line intensity ratios of the analytical lines to the internal standard lines were printed out for each step and exposure. These calculations were made for a maximum of 50 elements, four internal standard lines, and 11 exposures made with a seven-step sector.

The program is written in Fortran IV (version 13) and is operational on the IBM 7094-2/7044 direct-coupled system of the Lewis Research Center.

INTRODUCTION

In emission spectrographic analysis the concentrations of the various elements in a sample are determined from the photographic density of selected spectral lines that are recorded on a photographic plate. The conversion of the data from photographic density to concentration requires lengthy calculations and graphical procedures that are adaptable to automatic processing. The description of the graphical construction of the emulsion calibration curve from step-sectored spectra follows a standard practice as described in reference 1. The processing of the most laborious steps in the calculations by an electronic computer is the subject of this report.

The program, described in appendix B determines the emulsion calibration curve for each photographic plate and converts all percent transmissions to the intensity parameters from which element concentrations are derived. Calculations were made for a maximum of 50 elements, in a maximum of 11 samples. In spectral analysis using photographic photometry it is customary to stepwise attentuate the intensity of the spectral lines along their length to calibrate the emulsion and also to extend the concentration range for each exposure. This program allows the recording of data in a maximum of seven steps of atten-

uation for each spectral line. Conventionally, the element line intensities are ratioed to an internal standard line intensity to compensate for some experimental errors in the procedure. In this program provisions were made for calculating these ratios using a maximum of four internal standard line intensities. This was done to facilitate selection of internal standard lines in the development of analytical methods. A typical set of calculations, requiring about 40 hours when performed manually, may be completed in about 1 minute of computer time. In addition, the automatic calculations are less subject to error than those performed manually.

PHOTOGRAPHIC DATA REDUCTION

The conversion of photographic density to element concentration can be arbitrarily divided into four basic operations. Two of the operations are performed manually and two by computer as indicated:

(1) The conversion of photographic density into percent transmission using a densitometer (Manual)

(2) Graphical determination of the relation between percent transmission and the spectral line intensity that produced the photographic density, referred to as the emulsion calibration curve (ECC) (Computer)

(3) Calculation of the ratios of the analytical line intensities and the internal standard intensity, with appropriate background corrections (Computer)

(4) Graphical conversion of the line intensity ratios to elemental concentrations by means of calibration curves prepared from standards for each element sought (Manual)

The automation of the second operation, which involves the plotting of experimental data followed by two separate curve-fitting procedures, provides the emulsion calibration curve ECC. Although the mathematical relation for an emulsion calibration curve can be approximated in general by a mathematical function, a more precise procedure is to determine experimentally the ECC for each photographic plate. It should also be noted that the ECC is a function of the wavelength of the exciting light and for highest precision should therefore be determined for selected wavelength intervals. In the present work, however, a single ECC is determined representing an average over the experimental wavelength region. Additions can be made to this program to take into account this wavelength dependency should this be desired.

In the first curve-fitting procedure in operation (2), the percent transmission readings of adjacent steps of each spectral line recorded on card 3 (appendix A, fig. 1(b)), are input on linear X-Y coordinates. These ordered pairs (X,Y) have a definite intensity relation, known as the "step factor," which is determined by the physical configuration of the step sector used in the procedure to stepwise attenuate the light. In this work the step factor is 2.0 (i.e., any two adjacent steps of a given line have an intensity relation of 2.0). Similarly, alternate steps for a given line have an intensity

ratio of 2^2, and for steps separated by n step positions the intensity ratio of the darker step to the lighter step is 2^n. Thus, for the preliminary curve each ordered pair (X,Y) is derived from transmission readings for $n = 1$ (i.e., adjacent steps in the same line). It should be noted that these ordered pairs (X,Y) are derived from line, not background readings.

The program, as designed, orders a maximum of 250 pairs (X,Y) from the input data including two pairs fixed at (0,0) and (100,100), which are weighted to force the fit. Should the maximum number of ordered pairs exceed 250, it may be necessary to revise card 1 (appendix A, fig. 1(a)), so that the ordering of the elements will provide representative data with respect to wavelength region and to the range of densities in the first 250 ordered pairs. After calibration all of the input data are used in the ratio calculations.

The total number of points registered are curve fitted to a polynomial of the form

$$Y = A_1 + A_2X + A_3X^2 + A_4X^3$$

by a general least-squares method using the Crout reduction and a method developed at the Lewis Research Center by Bert Henry to invert the matrix. The resulting coefficients describe a curve known as a "preliminary emulsion calibration curve." This curve-fitting operation serves to effectively smooth all the plotted data.

The second curve-fitting operation results in the final emulsion calibration curve ECC, which relates percent transmission (ordinate) to the intensity parameter (abscissa). Values for plotting this curve are derived from the preliminary curve as follows: start at $X = 0.02$ (2 percent transmission) on the preliminary curve, and compute Y_1; now let $Y_1 = X_2$, and find Y_2 corresponding to this X_2 from the preliminary curve function. Then set $Y_2 = X_3$, and compute Y_3, . . . , etc. In this way a series of X's (maximum of 10) is generated, which represent the smoothed percent-transmission readings whose intensity relation are known from the step factor as explained previously. In the experiments presented herein this relation may be expressed as the percent transmission $T = 2^nZ$, where n is the difference in step number and Z is the intensity parameter that is related to element concentration in analytical work. The conversion of all percent-transmission data to this intensity parameter is done by a Lagrange four-point interpolation technique. The interpolation was easily performed on a large-scale computer and yielded greater accuracy than the method of least squares.

The programming of operation (3) requires the straightforward calculations of spectral line intensity ratios using the intensity parameters derived from the percent transmissions and the ECC, as described in operation (2). All intensity ratios were tabulated in both the background-corrected and the noncorrected forms; however, when background readings were not entered on card 3 (appendix A, fig. 1(b)), for either the internal standard or the analytical line, a zero was printed in the column reserved for the background-corrected ratio, as shown in the sample output for nickel (appendix C). In the calculation of line intensity ratios instructions are programmed so that maximum use

is made of the available data. For example, percent-transmission readings in a given exposure may not be recorded in the same step for the internal standard and the analytical lines. When this occurs, a calculation is made that automatically corrects for any step difference between the internal standard and the analytical lines. This calculation is performed by using 2^n as a multiplier, where 2 is the known step factor and n is the step difference. The intensity ratios obtained by this procedure may be subject to extrapolative errors; therefore, it is desirable to identify such values to warn of possible error by printing an asterisk to the right of the intensity ratios obtained by extrapolation. It should also be noted on the sample output (appendix C) that an average value is printed for each element and exposure. In the calculation of this average the extrapolated intensity ratios are given the same weight as the other intensity ratios. Although this may not be a statistically valid procedure, the error due to this simplification is not significant for most work at the Lewis Research Center.

Since a considerable amount of manual effort is still necessary to record the input data, errors in input can be expected to arise with about the same frequency as when calculations are made manually. The error-searching procedure is performed manually and is similar to the general procedure used by the spectrographer when making manual calculations. The preliminary curve is printed out, and wide deviations from the average are often recognized as erroneous data. The dubious value can then be traced back through the input, reread on the densitometer, and corrected if necessary. In addition, the percentage deviation of each of the data points from the preliminary curve fit is printed out in tabular form and serves as a useful means for revealing questionable data.

The line intensity ratios calculated by the program are then converted manually to element concentrations by means of calibration curves prepared from standards for each element sought. These calibrations cannot be conveniently programmed because the parameters under study at the Lewis Research Center affect the positions of the concentration curves. Once these calibrations are permanently established, the last operation, conversion of line intensity ratios to concentrations, can be included in the computer program by using curve fitting techniques similar to those described previously.

This program for spectrographic calculations forms a basis to which additional modifications can be made to make it more comprehensive. In its present state, the program serves the needs of a spectrographic laboratory engaged in both research and service analyses.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, November 23, 1965.

APPENDIX A

INPUT

This data reduction program is written in Fortran IV and is operational on the IBM 7094-2/7044 direct coupled system of the Lewis Research Center. The main program and its eight subroutines require $8000)_8$ store in common data, $30000)_8$ store for the program, and $25000)_8$ additional store for Lewis monitor systems routines. For a smaller computer installation, overlay or some other store-sharing technique would be necessary.

Figure 1 contains a list of the input with samples of the forms used at Lewis. The input in card type 3 is sorted in columns 11 to 7 to provide for the proper pairing of data in the preliminary curve fit.

The sample data (fig. 1) and the sample output (appendix C) are abbreviated to show only the first two internal standards and the element nickel.

Instructions for preparing the input are given in table I.

TABLE I. - INSTRUCTIONS FOR PREPARING INPUT

[See listing for specific formats.]

Card type	Number	Columns	Description of variables	
1 (Element data)	1	1 to 5	NEL	number of elements present (maximum, 50)
	NEL	7 to 12	EL	6 letter code for element
		19 to 24	ELB	6 letter code for element background
2 (Constants for one case)	1	2 to 5	NMAX	number percent transmissions recorded (maximum, 3850)
		10 to 15	PLATE	plate number
		16 and 17	KSTOP	number standards to be used (maximum, 4)
		18 and 19	NEXP	number exposures (maximum, 11)
	1	1 to 72	(DATE (I), I=1,12)	any statement about the data
3 (Data for one case)	NMAX	7 and 8	I	element number (must match order of type 1, 1 to 4 standards)
		9 and 10	J	exposure number
		11	K	step number (maximum, 7)
		13 to 18	CLU	percent transmission
		19 to 24	BAK	percent transmission of background

Card types 1 and 3 may be repeated for a number of cases, but card type 2 must be the same for all cases in a given run. Forms used at Lewis for card types 1 and 3 are shown in figure 1.

Column												
5|6	7	8	9	10	11	12	19	20	21	22	23	24
Element	Line identification						Background identification					
1	A		4	0	4	4	A		B	K	G	L
2	W		4	0	0	8	W		B	K	G	L
3	A	G	2	9	2	9	A	G	B	K	G	A
4	A	G	3	5	0	1	A	G	B	K	G	L
5	A	L	3	9	4	4	A	L	B	K	G	H
6	C	R	3	6	0	5	C	R	B	K	G	L
7	C	U	3	2	4	7	C	U	B	K	G	H
8	F	E	3	7	1	9	F	E	B	K	G	L
9	M	G	2	8	5	2	M	G	B	K	G	A
10	N	I	3	5	6	6	N	I	B	K	G	H
11	S	I	2	5	1	6	S	I	B	K	G	A
12	V		3	0	9	3	V		B	K	G	A
13	T	A	2	9	6	5	T	A	B	K	G	H
14	T	I	3	3	4	9	T	I	B	K	G	H
15	S	I	2	8	8	1	S	I	B	K	G	L
16	V		3	1	8	5	V		B	K	G	L
17	Z	R	3	3	9	1	Z	R	B	K	G	A
18	T	I	3	3	4	9	T	I	B	K	G	L
19	M	N	4	0	3	0	M	N	B	K	G	H
20	N	I	3	4	1	4	N	I	B	K	G	A
21	C	A	3	1	7	9	C	A	B	K	G	L
22	N	B	3	0	9	4	N	B	B	K	G	A
23	C	O	3	4	5	3	C	O	B	K	G	A
24	M	G	2	7	9	5	M	G	B	K	G	A
25	B	E	3	1	3	1	B	E	B	K	G	H
26	T	A	2	9	3	3	T	A	B	K	G	A

(a) Card type 1. Background measurements: L is measured on low wavelength side of line; H is measured on high wavelength side of line; A is measured as average of both sides of line.

SPECTROGRAPHIC PLATE READINGS

AUTOMATIC DATA PROCESSING WORKSHEET

(CARD TYPE 3)

NAME William A. Gordon

DATE August 1, 1965

PLATE NO. 705 PAGE 1

SAMPLE W - Re

ELEMENT NO. (7–8)	EXPOSURE NO. (9–10)	STEP NO. (11)	(12)	BLANK SPACE (13–14)	ELEMENT % TRANS-MISSION (15–18)	(19–20)	BACKGROUND % TRANS-MISSION (21–24)
1	1	3			7.7		
1	1	4			22.8		
1	1	5			53.3		
1	2	3			17.0		
1	2	4			42.0		
1	3	2			7.5		
1	3	3			22.0		
1	4	2			7.6		
1	4	3			22.0		
1	5	2			5.8		
1	5	3			18.9		
1	5	4			41.4		
1	6	2			14.0		
1	6	3			37.4		
1	7	2			6.9		
1	7	3			20.5		
1	8	3			21.8		
1	8	4			47.4		
2	1	1			76.0		79.0
2	2	6			13.4		
2	2	7			34.8		
2	3	6			8.0		
2	3	7			21.3		
2	4	5			8.6		
2	4	6			23.2		
2	4	7			50.4		
2	5	6			7.7		
2	5	7			20.3		
2	6	5			20.0		
2	6	6			48.1		
2	7	6			21.4		
2	7	7			46.7		
2	8	5			21.1		
2	8	6			45.3		

ELEMENT NO. (7–8)	EXPOSURE NO. (9–10)	STEP NO. (11)	(12)	BLANK SPACE (13–14)	ELEMENT % TRANS-MISSION (15–18)	(19–20)	BACKGROUND % TRANS-MISSION (21–24)
10	1	1			12.3		80.0
10	2	2			8.8		
10	2	3			20.7		
10	2	4			45.		
10	3	4			13.7		
10	3	5			28.6		
10	4	1			16.2		82.6
10	4	2			35.6		95.5
10	5	1			29.4		82.5
10	5	2			59.4		96.0
10	6	4			12.8		
10	6	5			28.5		
10	7	2			9.2		
10	7	3			19.3		
10	8	1			11.9		
10	8	2			26.7		

(b) Card type 3.

Figure 1. - Sample input.

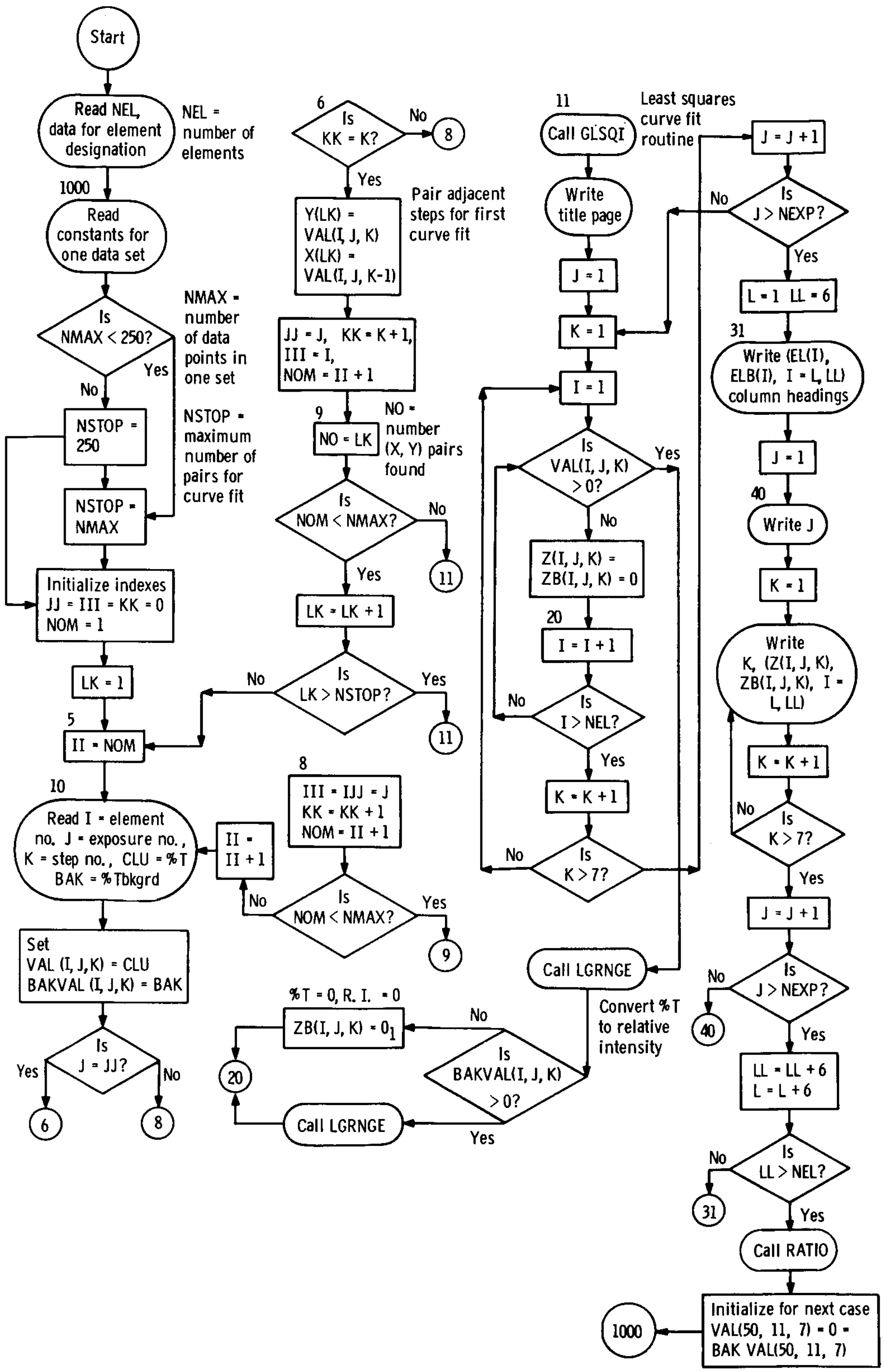
APPENDIX B

FORTRAN IV PROGRAM

A synopsis of the subroutines and their content listed in order of calling sequence is as follows:

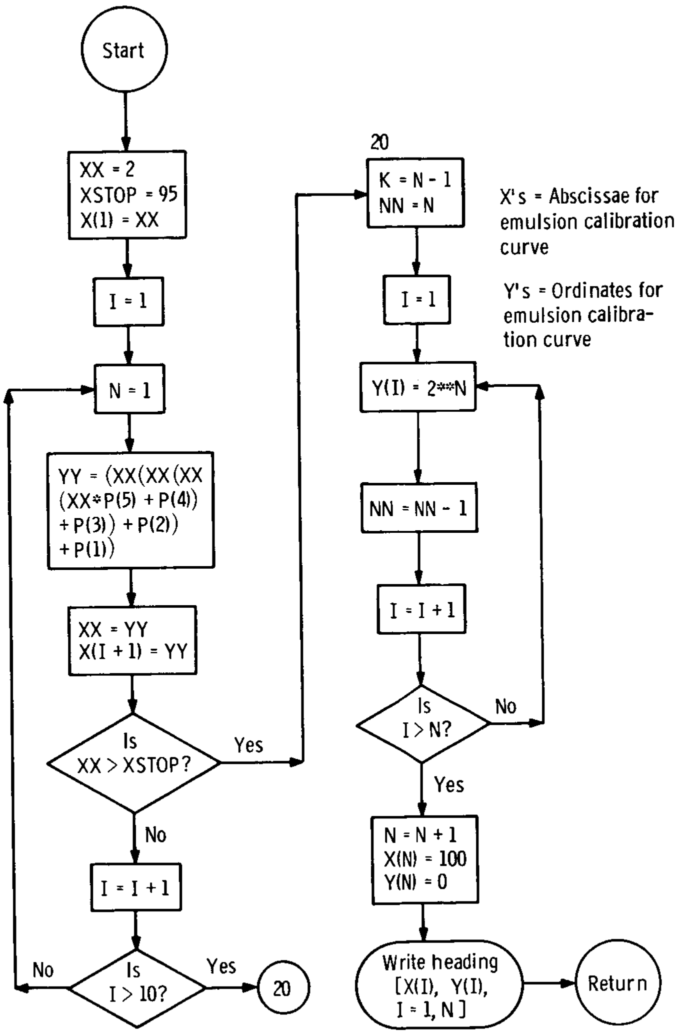
BEGIN	MAIN PROGRAM (1) Inputs data (2) Sets up X,Y-pairs for PC curve fit (3) Outputs relative intensities
GLSQ1	Performs a least-squares polynomial fit on X,Y-pairs
PLOTXY	Plots preliminary curve; PLOTXY is Lewis Monitor Subroutine (see ref. 2)
FUNC	Function Subprogram to generate independent variable function
BFUNC	Function Subprogram to backtransform independent variable function
DINVER	Subroutine using Crout reduction and a routine to invert matrix
DMVMUL	Subroutine to obtain solution vector from the inverse
CALC	Subroutine to determine X,Y-pairs for the ECC from the fitted PC
LGRNGE	Subroutine to perform four-point Lagrange interpolation; converts percent transmission to relative intensity
RATIO	Subroutine which ratios relative intensity of an element to that of a standard and corrects for background if necessary (maximum number of standards, 4)

Flow charts of BEGIN, CALC, and RATIO are shown in figure 2. These three routines are pertinent to the spectrographic data analysis. The remaining subroutines are in general use at the Lewis Research Center. The main program and subroutines used for data reduction are presented after figure 2.



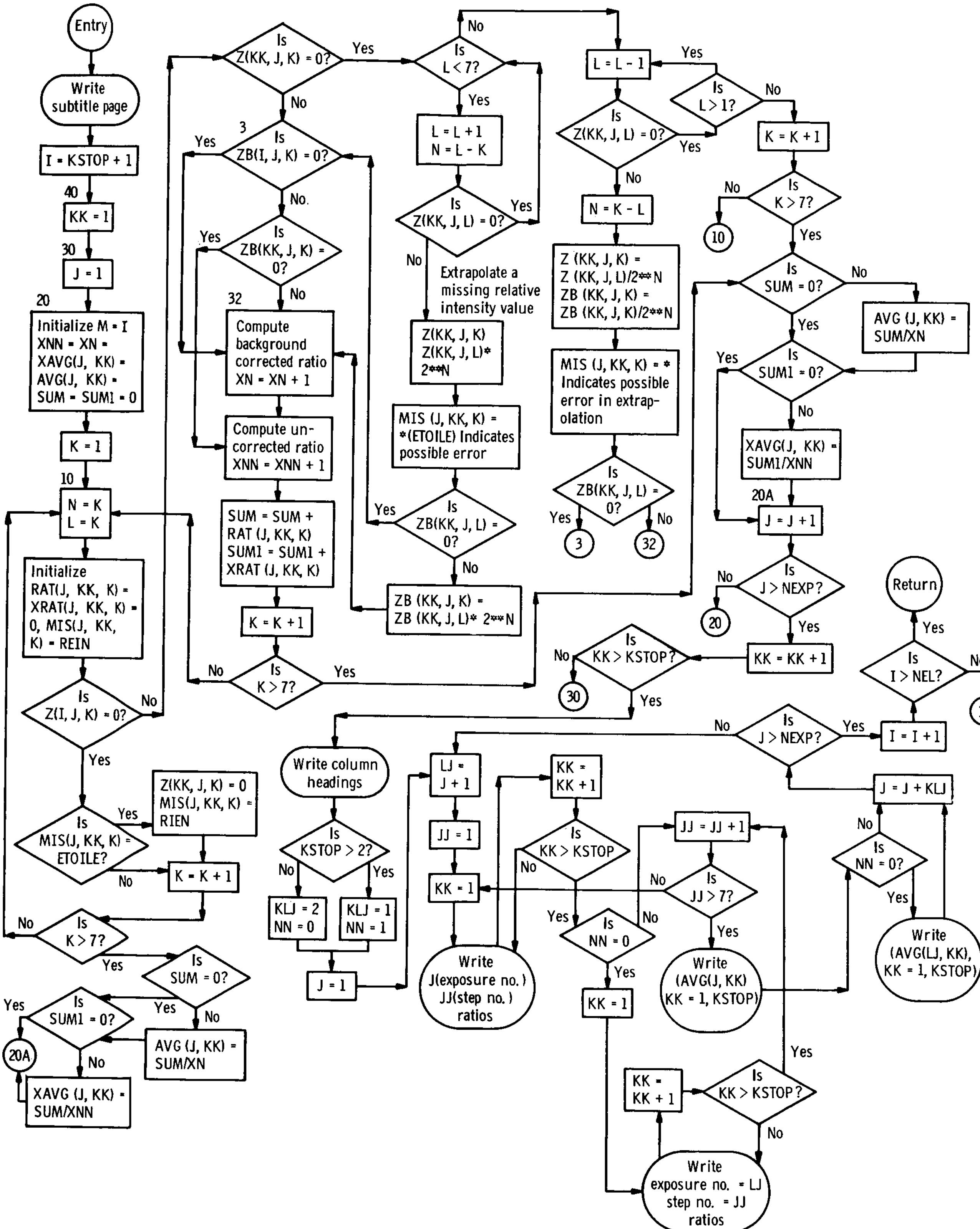
(a) Main program BEGIN.

Figure 2. - Flow charts.



(b) Subroutine CALC.

Figure 2. - Continued.



(c) Subroutine RATIO.

Figure 2. - Concluded.

```
$IBFTC BEGIN   LIST,DECK
C
C AUTOMATIC DATA PROCESSING FOR SPECTROGRAPHIC CALCULATIONS
      COMMON IW,KSTOP,NEXP
      COMMON Z(50,11,7),ZB(50,11,7)
      COMMON EL(50),ELB(50)
      DIMENSION VAL(50,11,7),BAKVAL(50,11,7),X(250),Y(500),P(35)
      DIMENSION ZX(200),ZY(200)
      DIMENSION DATE(12)
      EQUIVALENCE (Z,VAL) , (ZB,BAKVAL)
      READ(5,98) NEL
      DO 1 I=1,NEL
    1 READ(5,102)EL(I),ELB(I)
 1000 WRITE(6,106)
      READ(5,100) NMAX,PLATE,KSTOP,NEXP
      READ(5,99) (DATE(I),I=1,12)
C
C
C NMAX= NUMBER READINGS ON THIS PLATE
C
C   NEL= NUMBER OF ELEMENTS PRESENT IN THIS SAMPLE
C
C ELEMENTS INPUT FIRST (MAX=4) ARE TO BE USED AS INTERNAL STANDARDS.
C
C   AG AND AGX = SILVER, A=ARGON, W = TUNGSTEN.
C
C
C EL AND ELB ALLOW A MAXIMUM 6 CHARACTER DESIGNATION FOR EACH
C     ELEMENT AND ITS BACKGROUND TO BE USED AS COLUMN HEADINGS.  READIN
C     VALUE FOR - I - MUST MATCH ITS CODES IN EL(I), ETC)
C
      IF (NMAX-250)3,3,2
    2 NSTOP = 250
      GO TO 4
    3 NSTOP = NMAX
    4 JJ=0
      III = 0
      KK = 0
      NOM = 1
C BEGIN DETERMINATION OF POINTS TO BE USED IN FINDING THE PC
      DO  5 LK=1,NSTOP
      DO 10  II=NOM,NMAX
C
C  I= ELEMENT NUMBER, XX ,    INTEGER VALUE FROM 1 TO 50
C  J=EXPOSURE NUMBER, XX,     INTEGER VALUE FROM 1 TO 11
C  K= STEP NUMBER,  X,        INTEGER VALUE FROM 1 TO 7
C
C CLU = PERCENT T
C BAK = PERCENT T DUE TO BACKGROUND.
C
      READ (5,101) I,J,K,CLU,BAK
      VAL(I,J,K) = CLU
      BAKVAL(I,J,K) = BAK
      IF (JJ-J) 8,6,8
    6 IF (KK-K) 8,7,8
    7 Y(LK) = VAL(I,J,K)
      X(LK)= VAL(I,J,K-1)
      DEBUG LK,X(LK),Y(LK)
      NOM = II+1
      JJ = J
      KK = K+1
      III = I
```

```
      GO TO 9
    8 III=I
      JJ = J
      KK = K+1
      NOM=II+1
      IF(NOM-NMAX)10,10,9
   10 CONTINUE
    9 NO=LK
      IF (NOM-NMAX) 5,11,11
    5 CONTINUE
   11 CONTINUE
C  POINTS ARE AVAILABLE. CALL GLSQ1 TO DETERMINE PC
      IW=1
      CALL GLSQ1(X,Y,NO,P)
C PC HAS BEEN DETERMINED.  ECC HAS BEEN DEFINED.
      WRITE(6,106)
      WRITE(6,104) PLATE
      WRITE(6,105)
      WRITE(6,107) (DATE(I),I=1,12)
      KODE=1
C
C KODE = 1 INDICATES DERIVATIVE IS NOT TO BE CALCUALTED IN SUB. LGRNGE
C RENAME RESULTS OF SUB. CALC
      DO 15 J=1,NO
      ZX(J)=X(J)
   15 ZY(J)=Y(J)
C TRANSFORM PERCENT TS TO RELATIVE INTENSITIES BY MEANS OF LAGRANGE
C INTERPOLATION.
      DO 30 J=1,NEXP
      DO 25 K=1,7
      DO 20 I=1,NEL
      IF (VAL(I,J,K)-1.)16,16,17
   16 Z(I,J,K)=0.
      ZB(I,J,K)=0.
      GO TO 20
   17 CALL LGRNGE(ZX,ZY,NO,VAL(I,J,K),Z(I,J,K),DER,KODE)
      IF (BAKVAL(I,J,K)-1.)18,18,19
   18 ZB(I,J,K)=0.
      GO TO 20
   19 CALL LGRNGE(ZX,ZY,NO,BAKVAL(I,J,K),ZB(I,J,K),DER,KODE)
   20 CONTINUE
   25 CONTINUE
   30 CONTINUE
      L=1
      LL=6
C
C     PRINT RELATIVE INTENSITIES
C
   31 WRITE(6,108) (EL(I),ELB(I),I=L,LL )
      DO 50 J=1,NEXP
      WRITE(6,103) J
      DO 40 K=1,7
      WRITE(6,109) K,(Z(I,J,K),ZB(I,J,K),I=L,LL)
   40 CONTINUE
   50 CONTINUE
      LL=LL+6
      L=L+6
      IF (LL-NEL)51,51,52
   51 GO TO 31
C BEGIN FINDING RATIOS OF RELATIVE INTENSITIES.
   52 CALL RATIO (NEL,Z,ZB)
      WRITE(6,106)
```

```
      DO  70 I=1,7
      DO  65 J=1,11
      DO  60 K=1,50
      VAL(K,J,I)=0.
      BAKVAL(K,J,I)=0.
   60 CONTINUE
   65 CONTINUE
   70 CONTINUE
      GO TO 1000
C
C     FORMAT STATEMENTS
C
   98 FORMAT (I5)
   99 FORMAT (12A6)
  100 FORMAT(X,I4,4X,A6,2I2)
  101 FORMAT (6X,2I2,I1,X,2F6.2)
  102 FORMAT (6X,A6,6X,A6)
  103 FORMAT(4H EXP,I2)
  104 FORMAT(1H2,35X,45H SPECTROGRAPHIC  CALCULATIONS  FOR PLATE NO.   ,
     XA6)
  105 FORMAT(1H0,30X,62H  PER CENT TRANSMISSION  READINGS CONVERTED TO R
     XEL INTENSITY         )
  106 FORMAT(1H1)
  107 FORMAT(1H0,29X,12A6)
  108 FORMAT(1H1,6(A6,5X,A6,4X))
  109 FORMAT(1H ,I2,(12G10.3))
      STOP
      END
```

```
$IBFTC GLSWR    LIST,DECK,DEBUG                                         GLS00000
      SUBROUTINE GLSQ1(X,Y,NSMALL,P)                                    GLS00010
C                                                                       GLS00020
      COMMON IW                                                         GLS00030
      DIMENSION X(250),Y(500),D(35),A(35,35),ASAVE(35,35)               GLS00040
     1,P(35),P1(35),YCALC(250),DELY(250),XP(250),YP(500),ERRATA(250)    GLS00050
     2,ELM(2),TITLE(12),FMT(12),FMTO(12),W(250)                         GLS00060
      DIMENSION AIN(35,35)                                              GLS00070
      DIMENSIUN FMTW(7),KMTW(7),PK(1),KPL(15),CC(35)                    GLS00080
      EQUIVALENCE (FMTW(5),KMTW(5))                                     GLS00090
      DATA (FMTW(I),I=1,7)/6H(22HO ,6HTHE PA,6HRAMETE,6HRS (AO,6H-A I2,,GLS00100
     16H5H) AR,3HE )/,KMT51,KMT52/6H-A I1,,6H-A I2,/                    GLS00110
      DATA(TITLE(I),I=1,12)/6HAUTOMA,6HTIC DA,6HTA PRO,6HCESSIN,6HG FOR GLS00120
     X,6HSPECTR,6HOGRAPH,6HIC CAL,6HCULATI,6HONS    ,6H      ,6H      / GLS00130
C                                                                       GLS00140
C  MAIN PROGRAM FOR LEAST SQUARES ANALYSIS HAS BEEN ALTERED FOR THIS    GLS00150
C SPECIFIC PROBLEM.                                                     GLS00155
C                                                                       GLS00160
C ALL THE OPTIONS IN THE ORIGINAL PROGRAM HAVE BEEN REMOVED.            GLS00170
      DOUBLE PRECISION A,D,CC,DXMAX,AIN                                 GLS00180
      PK(1)=1.0                                                         GLS00190
      KPL=64                                                            GLS00200
      KPL(2)=2                                                          GLS00210
      POOL1=0.                                                          GLS00220
      POOL2=0.                                                          GLS00230
      NFMTO=NBIG*3 - 2                                                  GLS00240
      NBIG=4                                                            GLS00250
      IPL=1                                                             GLS00260
      IY=0                                                              GLS00270
      NBIGSV=NBIG                                                       GLS00280
C                                                                       GLS00290
C    NSMALL=NO. OF DATA POINTS --- NBIG=NO. OF COEFFICIENTS DESIRED     GLS00300
C  THE ORIGINAL DATA IS PLOTTED                                         GLS00310
C IF IT BECOMES DESIRABLE TO OMIT THE PLOT CHANGE IPL TO 0              GLS00320
      NNN=NBIG                                                          GLS00330
      MAX =35                                                           GLS00340
      DO 32 I=1,NSMALL                                                  GLS00350
   32 W(I)=1.                                                           GLS00360
      NSMALL=NSMALL+2                                                   GLS00370
      NN=NSMALL                                                         GLS00380
      X(NN-1)=0.                                                        GLS00390
      Y(NN-1)=0.                                                        GLS00400
      X(NN)=100.                                                        GLS00410
      Y(NN)=100.                                                        GLS00420
      W(NN)=50.                                                         GLS00430
      W(NN-1)=50.                                                       GLS00440
      KKK=1                                                             GLS00450
      SN=NSMALL                                                         GLS00460
 6000 DO 6010 I=1,NSMALL                                                GLS00470
      XP(I)=X(I)                                                        GLS00480
 6010 YP(I)=Y(I)                                                        GLS00490
C                                                                       GLS00500
      NBIG=NBIGSV                                                       GLS00510
      NSAME=NSAMSV                                                      GLS00520
      SUMYP=0.                                                          GLS00530
      XMAXX=0.                                                          GLS00540
      DO 501 I=1,NSMALL                                                 GLS00550
      IF (XMAXX-ABS(X(I))) 33,501,501                                   GLS00560
   33 XMAXX=ABS(X(I))                                                   GLS00570
      DXMAX=XMAXX                                                       GLS00580
  501 CONTINUE                                                          GLS00590
```

```
      DO 20 I=1,NSMALL
      X(I)=X(I)/XMAXX
      XP(I)=X(I)
      YP(I)=Y(I)
   20 SUMYP=SUMYP+YP(I)
 1903 SUMY=0.
      CN=NBIG
      KN=NBIG-1
      DETNUM=0.
      DETDEN=0.
      YPMEAN=SUMYP/SN
      YMEAN=YPMEAN
C
C
      DO 23 I=1,NSMALL
      IF(IY) 22,23,22
   22 Y(I)=FUNC(IY,Y(I))
   23 SUMY=SUMY+Y(I)
      YMEAN=SUMY/SN
C
C             SET UP THE MATRIX OF COEFFICIENTS
C
      DO 2 I=1,NBIG
      DO 2 J=1,NBIG
      A(I,J)=0.
      DO 2 K=1,NSMALL
      FI=FUNC(I,X(K))
      FJ=FUNC(J,X(K))
      IF (IW) 35,36,35
   35 A(I,J)=A(I,J)+FI*FJ*W(K)
      GO TO 2
   36 A(I,J)=A(I,J)+FI*FJ
    2 CONTINUE
C
      DO 14 I=1,NBIG
      D(I)=0.
      DO 14 K=1,NSMALL
      FI=FUNC(I,X(K))
      IF (IW) 37,38,37
   37 D(I)=D(I)+Y(K)*FI*W(K)
      GO TO 14
   38 D(I)=D(I)+Y(K)*FI
   14 CONTINUE
C
      WRITE (6,397) TITLE
  397 FORMAT(1H1,10X,12A6)
C
  300 CALL DINVER (A,NNN,AIN,MAX,DET,ERR,D)
      CALL DMVMUL(AIN,NNN,D,CC,MAX)
      XXAXX=1./XMAXX
      DO 301 J=1,NBIG
      P(J)=CC(J)
  301 P(J)=P(J)*FUNC(J,XXAXX)
C
C     COMPUTE Y-CALC,DELTA-Y,AND STANDARD DEVIATION
C
  130 CONTINUE
      DEBUG (P(J),J=1,NBIG)
      ERS=0.
      DEV=0.
      DO 8 I=1,NSMALL
      X(I)=X(I)*XMAXX
```

```
      K=NSMALL+I                                                        GLS01220
      Y(K)=0.                                                           GLS01230
      DO 9 J=1,NBIG                                                     GLS01240
      FJ=FUNC(J,X(I))                                                   GLS01250
      DEBUG FJ                                                          GLS01260
    9 Y(K)=Y(K)+P(J)*FJ                                                 GLS01270
      TEM=Y(I)-YMEAN                                                    GLS01280
      DETDEN=DETDEN+TEM*TEM                                             GLS01290
      TEM=Y(K)-YMEAN                                                    GLS01300
      DETNUM=DETNUM+TEM*TEM                                             GLS01310
      DELY(I)=Y(I)-Y(K)                                                 GLS01320
      ERRATA(I)=DELY(I)/Y(K)*100.                                       GLS01330
      ERS=ERS+ERRATA(I)**2                                              GLS01340
    8 DEV=DEV+DELY(I)*DELY(I)                                           GLS01350
      POOL1=POOL1+DEV                                                   GLS01360
      ENDIV=SN-CN-1.                                                    GLS01370
      TVRDEN=TVRDEN+ENDIV                                               GLS01380
      TVRNUM=POOL1                                                      GLS01390
  100 DEV=DEV/ENDIV                                                     GLS01400
      DVTN=SQRT(DEV)                                                    GLS01410
      ERS=ERS/SN                                                        GLS01420
      ERA=SQRT(ERS)                                                     GLS01430
      TOTVAR=TVRNUM/TVRDEN                                              GLS01440
      TOTDEV=SQRT(TOTVAR)                                               GLS01450
      DETRM=DETNUM/DETDEN                                               GLS01460
      CORRL=SQRT(DETRM)                                                 GLS01470
      WRITE(6,401)                                                      GLS01480
      DO 10 I=1,NSMALL                                                  GLS01490
      K=NSMALL+I                                                        GLS01500
   10 WRITE(6,402) X(I),Y(I),Y    (K),DELY(I),ERRATA(I)                 GLS01510
      WRITE(6,406)                                                      GLS01520
  406 FORMAT(41HOTHE REGRESSION EQUATION FOR THE ABOVE IS /1H0,35H Y = AGLS01530
     XO + A1*X + A2*X**2 + A3*X**3        )                             GLS01540
  409 IF (KN-10) 407,405,405                                            GLS01550
  405 KMTW(5)=KMT52                                                     GLS01560
      GO TO 408                                                         GLS01570
  407 KMTW(5)=KMT51                                                     GLS01580
  408 WRITE (6,FMTW) KN                                                 GLS01590
      WRITE (6,403) (P(I),I=1,NBIG)                                     GLS01600
      WRITE (6,404) DEV,DVTN,DETRM,CORRL,TOTVAR,TOTDEV,ERS,ERA          GLS01610
      WRITE (6,91) DET                                                  GLS01620
   91 FORMAT(13HODETERMINANT= G14.6//)                                  GLS01630
      IF(IW) 422,419,422                                                GLS01640
  422 WRITE(6,430)                                                      GLS01650
      DO 420 I=1,NSMALL                                                 GLS01660
      IF (W(I)-1.) 421,420,421                                          GLS01670
  421 WRITE(6,431)X(I),Y(I),W(I)                                        GLS01680
  420 CONTINUE                                                          GLS01690
  419 CONTINUE                                                          GLS01700
  431 FORMAT(1H ,2X,2HX=G15.6,2X,2HY=G15.6,2X,12HWITH WEIGHT= F7.0)     GLS01710
  430 FORMAT(44HOTHE ABOVE DATA HAS BEEN WEIGHTED AS FOLLOWS   )        GLS01720
  401 FORMAT(1H0,2X,10H IND. VAR. ,8X,10H DEP.VAR. ,8X,12HCALC. FUNC.   GLS01730
     X,6X,10H DEVIATION,8X,15H PER CENT ERROR    )                      GLS01740
  402 FORMAT(1H ,(5(F12.4,6X)))                                         GLS01750
  403 FORMAT(7G18.8)                                                    GLS01760
  404 FORMAT(1H0,2X,14H THE VARIANCE=G15.7,20H STANDARD DEVIATION=G15.7/GLS01770
     13X,14HDETERMINATION=G15.7,8X,12HCORRELATION=G15.7/17H POOLED VARIAGLS01780
     2NCE=G15.7,3X,17HPOOLED DEVIATION=G15.7/                           GLS01790
     3       1H0,2X,14H PCT VARIANCE=G15.7,20H STD. PCT DEVIATION=G15.7)GLS01800
      GO TO (101,102),KKK                                               GLS01810
  101 DO 24 I=1,NSMALL                                                  GLS01820
      K=NSMALL+I                                                        GLS01830
```

```
      IF (IY) 25,26,25
   25 YP(K)=BFUNC(IY,Y(K))
      GO TO 24
   26 YP(K)=Y(K)
   24 CONTINUE
      IF (IPL-1)  29,803,801
  803 KKK=2
  801 CONTINUE
      KPL(3)=NSMALL
      K2N=NSMALL+NSMALL
  102 WRITE(6,77)TITLE
   77 FORMAT(2HPT,12A6/2HPT/2HPT,59X,7HNOTE---/2HPT/2HPT,59X,28HORIGINAL
     1 DATA PLOTTED WITH • /2HPT,59X,30HCALCULATED DATA PLOTTED WITH + /
     X2HPT/2HPT,59X,14HPLOT OF PC       )
      CALL SCALE(NSMALL,X,KKLU)
      CALL SCALE(K2N,Y ,KKLY)
      CALL PLOTMY(X ,Y ,KPL,PK)
      WRITE(6,78)
   78 FORMAT(2HPL,59X,23HLIGHT STEP VS DARK STEP    )
  802 CONTINUE
      GO TO (103,29),KKK
  103 CONTINUE
   27 DEV=0.
      DETNUM=0.
      DETDEN=0.
      DO 28 I=1,NSMALL
      K=NSMALL +I
      X(I)=XP(I)
      Y(I)=YP(I)
      Y(K)=YP(K)
      TEM=Y(I)-YPMEAN
      DETDEN=DETDEN+TEM*TEM
      TEM=Y(K)-YPMEAN
      DETNUM=DETNUM+TEM*TEM
      DELY(I)=Y(I)-Y(K)
      ERRATA(I)=DELY(I)/YP(K)
   28 DEV=DEV+DELY(I)*DELY(I)
      POOL2=POOL2+DEV
      TVRNUM=POOL2
      KKK=2
      GO TO 100
   29 CALL CALC (XP,YP,NSMALL,NBIG,P)
       DO 6 I=1,NSMALL
      X(I)=XP(I)
       Y(I)=YP(I)
    6 CONTINUE
      RETURN
      END
```

```
$IBFTC FLINFN  LIST,DECK
C FUNCTION SUBROUTINE TO GENERATE INDEPENDENT VARIABLE FUNCTIONS
      FUNCTION FUNC (I,X)
      Z=X
      K=I
C
C  THE NUMBER OF THE STATEMENT IS IDENTICAL TO THE  NUMBER OF THE TERM
C    IN THE POLYNOMIAL TO BE FITTED.
C
      IF (K-6) 100,6,7
    7 WRITE (6,10) K
   10 FORMAT(1H0,5X,72HTOO MANY COEFFICIENTS ASKED FOR - ONLY  6  ARE AV
     1AILABLE YOU CANNOT GET   I3)
      STOP
    6 ANS=ALOG10(Z)
      GO TO 99
  100 IF (K-4) 101,4,5
    5 ANS=Z*Z
      ANS=ANS*ANS
      GO TO 99
    4 ANS=Z*Z*Z
      GO TO 99
  101 IF (K-2) 1,2,3
    3 ANS=Z*Z
      GO TO 99
    2 ANS=Z
      GO TO 99
    1 ANS=1.
   99 FUNC=ANS
      RETURN
      END
```

```
$IBFTC BLINFN  LIST,DECK
C SUBROUTINE TO BACK-TRANSFORM  Y(I) ARRAY
      FUNCTION BFUNC (I,X)
      Z=X
      K=I
C
C   THE NUMBER OF THE STATEMENT IS THE NUMBER TO BE USED IN SPECIFYING
C     THE TYPE OF CONVERSION.
C      IT MUST AGREE WITH THE CONVERSION USED IN SUBROUTINE FUNC.
C
      IF (K-6) 100,6,7
    7 WRITE (6,10) K
   10 FORMAT(1H0,5X,44HWRONG BACK-TRANSFORMATION OF Y REQUESTED, K=   I3)
      STOP
    6 ANS=10.**Z
      GO TO 99
  100 IF (K-4) 101,4,5
    5 ANS=SQRT(Z)
      ANS=SQRT(ANS)
      GO TO 99
    4 ANS=Z**.333333333
      GO TO 99
  101 IF (K-2) 1,2,3
    3 ANS=SQRT(Z)
      GO TO 99
    2 ANS=Z
      GO TO 99
    1 ANS=1.
   99 BFUNC=ANS
      RETURN
      END
```

```
$IBFTC DINV    LIST,DECK,DEBUG
C SUBR USING CROUT REDUCTION AND HENRY INVERSE ROUTINE
      SUBROUTINE DINVER(B,NNN,A,MAX,DET,ERR,D)
      DIMENSION A(MAX,MAX),B(MAX,MAX),D(MAX),AN(60)
      DOUBLE PRECISION A,B,D,AN
      KM1=NNN
      MM1=KM1-1
      MP1=KM1+1
      DO 25 I=1,KM1
      A(I,MP1)=D(I)
      DO 25 J=1,KM1
   25 A(I,J)=B(I,J)
      DO 15 N=2,MP1
   15 A(1,N)=A(1,N)/A(1,1)
      DO 7 J=2,MP1
      M=0
      L=J-1
      DO 7 I=2,KM1
      M=M+1
      IF(M-L) 10,10,9
    9 M=L
   10 DO 6 N=1,M
    6 A(I,J)=A(I,J)-A(N,J)*A(I,N)
      IF(I-J) 12,7,7
   12 A(I,J)=A(I,J)/A(I,I)
    7 CONTINUE
      DO11 II=1,KM1
      DEBUG(A(II,JJ),JJ=1,MP1)
   11 CONTINUE
      DET=1.0
      DO 2 I=1,KM1
      B(I,MP1)=A(I,I)*A(I,MP1)**2
      DET=DET*A(I,I)
    2 A(I,I)=1./A(I,I)
      DO 3J=1,MM1
      N=J+1
      DO 4I=N,KM1
      KJ=J
      MJ=I-N
      A(I,J)=A(I,J)*A(J,J)
      IF(MJ) 4,4,5
    5 DO 16 K=1,MJ
      KJ=KJ+1
   16 A(I,J)=A(I,J)+A(I,KJ)*A(KJ,J)
    4 A(I,J)=-(A(I,J)*A(I,I))
    3 CONTINUE
      DO 17 J=1,MM1
      KJ=KM1-J
      DO 8 I=1,KJ
      DO 8 K=1,J
      KK=MP1-K
    8 A(KJ,I)=A(KJ,I)-A(KJ,KK)*A(KK,I)
   17 CONTINUE
      DO 19 J=1,MM1
      KK=KM1-J
      KJ=MP1-J
      DO 110 I=KJ,KM1
  110 A(MP1,I)=A(KK,I)
      DO 111 K=KJ,KM1
      A(KK,K)=0.
      DO 111 L=KJ,KM1
```

```
111 A(KK,K)=A(KK,K)-A(MP1,L)*A(L,K)                                DIN00610
 19 CONTINUE                                                        DIN00620
    DO 88 II=1,KM1                                                  DIN00630
    DEBUG(A(II,JJ),JJ=1,MP1)                                        DIN00640
 88 CONTINUE                                                        DIN00650
    REWIND 7                                                        DIN00660
    WRITE (7) ((B(I,J),I=1,KM1),J=1,KM1)                            DIN00670
    DO 114 I=1,KM1                                                  DIN00680
    DO 112 J=1,KM1                                                  DIN00690
    AN(J)=0.                                                        DIN00700
    DO 112 K=1,KM1                                                  DIN00710
112 AN(J)=AN(J)+B(I,K)*A(K,J)                                       DIN00720
    DO 114 II=1,KM1                                                 DIN00730
    B(I,II)=(-AN(II))                                               DIN00740
    IF (II-I) 114,113,114                                           DIN00750
113 B(I,II)=B(I,II)+1.                                              DIN00760
114 CONTINUE                                                        DIN00770
    DO 117 I=1,KM1                                                  DIN00780
    DO 115 J=1,KM1                                                  DIN00790
    AN(J)=0.                                                        DIN00800
    DO 115 K=1,KM1                                                  DIN00810
115 AN(J)=AN(J)+A(I,K)*B(K,J)                                       DIN00820
    DO 116 II=1,KM1                                                 DIN00830
116 A(I,II)=A(I,II)+AN(II)                                          DIN00840
117 CONTINUE                                                        DIN00850
    DO 18 II=1,KM1                                                  DIN00860
    DEBUG(A(II,JJ),JJ=1,MP1)                                        DIN00870
    DEBUG(B(II,JJ),JJ=1,MP1)                                        DIN00880
 18 CONTINUE                                                        DIN00890
    REWIND 7                                                        DIN00900
    READ  (7) ((B(I,J),I=1,KM1),J=1,KM1)                            DIN00910
    ERR=0.                                                          DIN00920
    DO 20 I=1,KM1                                                   DIN00930
    DO 20 K=1,KM1                                                   DIN00940
    ERR1=0.                                                         DIN00950
    DO 21 J=1,KM1                                                   DIN00960
 21 ERR1=B(I,J)*A(J,K)+ERR1                                         DIN00970
    IF (I-K) 23,22,23                                               DIN00980
 22 ERR1=1.-ERR1                                                    DIN00990
 23 ERR1=ABS(ERR1)                                                  DIN01000
    IF (ERR-ERR1) 24,20,20                                          DIN01010
 24 ERR=ERR1                                                        DIN01020
 20 CONTINUE                                                        DIN01030
    RETURN                                                          DIN01040
    END                                                             DIN01050
```

```
$IBFTC DSLV    LIST,DECK,DEBUG
C SUBROUTINE TO OBTAIN SOLUTION VECTOR FROM INVERSE B
C
C SOLUTION VECTOR IS RETURNED IN THE AN ARRAY AND IN ((B(I,NP1),I=1,NNN)
C WHICH IS THE AUGMENTED MATRIX INVERTED
C
      SUBROUTINE DMVMUL(B,NNN,D,AN,MAX)
      DIMENSION B(MAX,MAX),D(MAX),AN(MAX)
      DOUBLE PRECISION B,D,AN
      M=NNN
      NP1=NNN+1
      DO 100  I=1,M
      AN(I)=0.
      DO 100 J=1,M
  100 AN(I)=B(I,J)*D(J)+AN(I)
      DO11 II=1,M
      DEBUG(B(II,JJ),JJ=1,M)
   11 CONTINUE
      DEBUG(AN(II),II=1,M)
      DO 4 I=1,NNN
    4 B(I,NP1)=AN(I)
      WRITE (6,15)
      DO 14 J=1,M
      DO 13 I=1,M
   13 B(MP1,I)=B(I,J)/SQRT(B(I,I)*B(J,J))
   14 WRITE (6,16)(B(MP1,K),K=1,M)
   15 FORMAT(20H0CORRELATION MATRIX=    )
   16 FORMAT(1H08G16.8)
      RETURN
      END
```

```
$IBFTC CAL     LIST,DECK                                                 CAL00000
      SUBROUTINE CALC(X,Y,N,K,P)                                         CAL00010
C                                                                        CAL00020
C DETERMINE AN EMULSION CALIBRATION CURVE FOR INPUT TO  LAGRANGE         CAL00030
C                     INTERPOLATION ROUTINE.                             CAL00040
      COMMON IW                                                          CAL00050
      DIMENSION X(250),Y(500),P(35)                                      CAL00060
    1 XX=2.                                                              CAL00070
      XSTOP=95.                                                          CAL00080
      X(1)=XX                                                            CAL00090
      DO 10 I=1,10                                                       CAL00100
      N=I                                                                CAL00110
      YY=P(1)+P(2)*XX+P(3)*XX**2+P(4)*XX**3 +P(5)*XX**4                  CAL00120
      XX=YY                                                              CAL00130
      X(I+1)=YY                                                          CAL00140
      IF (XX-XSTOP) 10,10,20                                             CAL00150
   10 CONTINUE                                                           CAL00160
   20 K=N-1                                                              CAL00170
      NN=N                                                               CAL00180
    4 DO 30 I=1,N                                                        CAL00190
      Y(I)=2.**NN                                                        CAL00200
      NN=NN-1                                                            CAL00210
   30 CONTINUE                                                           CAL00220
      N=N+1                                                              CAL00230
      X(N)=100.                                                          CAL00240
      Y(N)=0.                                                            CAL00250
      WRITE(6,99)                                                        CAL00260
      WRITE(6,103) (X(I),Y(I),I=1,N)                                     CAL00270
   99 FORMAT(1H0,100H     X     VS.     Y     (DEFINES EMULSION CALIBRATION CAL00280
     XCURVE)  FOR INPUT TO LAGRANGE ROUTINE.                    )        CAL00290
  103 FORMAT(1H0,2F10.4)                                                 CAL00300
      IW=0                                                               CAL00310
  101 RETURN                                                             CAL00320
      END                                                                CAL00330
```

```
$IBFTC LGRN     LIST,DECK,DEBUG
      SUBROUTINE LGRNGE(X,Y,N,ARG,ANS,DER,KODE)
      DIMENSION X(200),Y(200),A(10),C(4)
      EQUIVALENCE (XX,A(1)),(X0,A(2)),(X1,A(3)),(X2,A(4)),(X3,A(5)),
     1(Y0,A(6)),(Y1,A(7)),(Y2,A(8)),(Y3,A(9)),(C1,C(1)),(C2,C(2)),(C3,C(
     23)),(C4,C(4))
      IF(ARG-X(2))10,10,11
   10 MX=1
      GO TO 51
   11 IF(ARG-X(N-1)) 12,12,13
   13 MX=N-3
      GO TO 51
   12 K=N-1
      DO 14 JA=2,K
      IF(ARG-X(JA))15,15,14
   15 MX=JA-2
      GO TO 51
   14 CONTINUE
   51 IF(KODE-1)1,2,1
    1 CON=0.0
      GO TO 50
    2 CON=1.
   50 XX=ALOG(ARG+CON)
      DO 3 I=1,4
      MXI=MX+I-1
      A(I+1)=ALOG(X(MXI)+CON)
    3 A(I+5)=ALOG(Y(MXI)+CON)
      DEBUG XX,X0,X1,X2,X3
      ANS=((XX-X1)*(XX-X2)*(XX-X3)/((X0-X1)*(X0-X2)*(X0-X3)))*Y0 +(XX-X0
     1)*(XX-X2)*(XX-X3) *Y1/((X1-X0)*(X1-X2)*(X1-X3)) +(XX-X0)*(XX-X1)*
     2(XX-X3)*Y2/((X2-X0)*(X2-X1)*(X2-X3))+(XX-X0)*(XX-X1)*(XX-X2)*Y3/
     3((X3-X0)*(X3-X1)*(X3-X2))
      ANS=EXP(ANS)-CON
      DEBUG ANS
      GO TO (5,4),KODE
    4 DO 7 I=2,5
    7 C(I-1)=XX-A(I)
      CC0=Y0/(X0-X1)/(X0-X2)/(X0-X3)
      CC1=Y1/(X1-X0)/(X1-X2)/(X1-X3)
      CC2=Y2/(X2-X0)/(X2-X1)/(X2-X3)
      CC3=Y3/(X3-X0)/(X3-X1)/(X3-X2)
      DER=ANS/ARG*(CC0*(C2*C3+C2*C4+C3*C4)+CC1*(C1*C3+C1*C4+C3*C4)+CC2*(
     1C1*C2+C1*C4+C2*C4)+CC3*(C1*C2+C1*C3+C2*C3))
    5 RETURN
      END
```

```
$IBFTC RAT     LIST,DECK                                                 RAT00000
       SUBROUTINE FATIO (NEL,Z,ZB)                                       RAT00010
C                                                                        RAT00020
C      COMPUTES RATIO  OF RELATIVE INTENSITY OF AN ELEMENT TO RELATIVE   RAT00030
C      INTENSITY OF A STANDARD, MAXIMUM NUMBER OF STANDARDS IS FOUR,     RAT00040
C      MAXIMUM NUMBER OF ELEMENTS IS FIFTY.                              RAT00050
C                                                                        RAT00060
      REAL MIS                                                           RAT00070
      COMMON IW,KSTOP,NEXP                                               RAT00080
      COMMON Z(50,11,7),ZB(50,11,7)                                      RAT00090
      COMMON EL(50)                                                      RAT00100
      DIMENSION RAT (11,4,7),XRAT(11,4,7),AVG(11,4),XAVG(11,4)           RAT00110
      DATA RIEN,ETOILE/6H      ,3H*  /                                   RATC1200
      DIMENSION MIS(11,4,7)                                              RAT00130
      WRITE(6,98)                                                        RAT00140
      WRITE(6,99)(FL(I),I=1,KSTOP       )                                RAT00150
      WRITE(6,101)                                                       RAT00160
      WRITE(6,105)                                                       RAT00170
      WRITE(6,106)                                                       RAT00180
      KST=KSTOP+1                                                        RAT00190
      DO 40 I=KST,NEL                                                    RAT00200
      DO 30 KK=1,KSTOP                                                   RAT00210
      DO 20 J=1,NEXP                                                     RAT00220
      M=I                                                                RAT00230
      XN=0.                                                              RAT00240
      XNN=0.                                                             RAT00250
      XAVG(J,KK)=0.                                                      RAT00260
       AVG(J,KK)=C.                                                      RAT00270
      SUM=0.                                                             RAT00280
      SUM1=0.                                                            RAT00290
      DO 10  K = 1,7                                                     RAT00300
      N=K                                                                RAT00310
      L=K                                                                RAT00320
      RAT(J,KK,K)=0.                                                     RAT00330
      XRAT(J,KK,K)=0.                                                    RAT00340
      IF(I-KST)1,4,1
    4 MIS(J,KK,K)=RIEN
C                                                                        RAT00360
C      ARRAY MIS SHOWS PROGRAM EXTRAPOLATED A REL INTENSITY  IF THERE WASRAT00370
C      NO ORIGINAL DATA FOR THAT EXPOSURE AND STEP.                      RAT00380
C                                                                        RAT00390
    1 IF (Z(I,J,K))2,6,2
    6 IF (MIS(J,KK,K)-ETOILE)10,7,10
    7 Z(KK,J,K)=0.
      MIS(J,KK,K)=RIEN
      GO TO 10
    2 IF (Z(KK,J,K)) 3,11,3                                              RAT00410
C TEST FOR BACKGROUND                                                    RAT00420
    3 IF (ZB(I,J,K)) 32,5,32                                             RAT00430
    5 IF (ZB(KK,J,K)) 32,31,32                                           RAT00440
C IF IN STEP 7 GO TO 21 AND START SEARCHING LOWER STEPS.                 RAT00450
C IF NOT IN STEP 7 START SEARCHING HIGHER STEPS.                         RAT00460
   11 IF (L-7) 12,21,21                                                  RAT00470
   12 L = L+1                                                            RAT00480
      N=L-K                                                              RAT00490
      IF(Z(KK,J,L)) 13,11,13                                             RAT00500
C CORRECT FOR STEP MOVEMENTS                                             RAT00510
   13 Z(KK,J,K) = Z(KK,J,L) * 2.**N                                      RAT00520
      MIS(J,KK,K)=ETOILE                                                 RAT00530
   14 IF (ZB(KK,J,L)) 15,3,15                                            RAT00540
   15 ZB(KK,J,K) = ZB(KK,J,L) * 2.**N                                    RAT00550
      GO TO 32                                                           RAT00560
C START SEARCH OF LOWER STEPS                                            RAT00570
```

```
   21 IF (L-7) 11,22,22                                              RAT00580
   22 L = L-1                                                        RAT00590
      IF(Z(KK,J,L)) 23,27,23                                         RAT00600
   23 N = K-L                                                        RAT00610
C CORRECT FOR STEP MOVEMENT                                           RAT00620
      Z(KK,J,K)=Z(KK,J,L)/2.**N                                      RAT00630
      MIS(J,KK,K)=ETOILE                                             RAT00640
      ZB(KK,J,K)=ZB(KK,J,L)/2.**N                                    RAT00650
      IF(   ZB(KK,J,L)) 32,3,32                                      RAT00660
   27 IF (L-1) 10,10,22                                              RAT00670
C DETERMINE RATIO                                                     RAT00680
   32 RAT(J,KK,K) = (Z(I,J,K) - ZB(I,J,K))/(Z(KK,J,K) - ZB(KK,J,K))  RAT00690
      XN=XN+1.                                                       RAT00700
   31 XRAT(J,KK,K) = Z(I,J,K) / Z(KK,J,K)                            RAT00710
      XNN=XNN+1.                                                     RAT00720
   33 SUM = SUM + RAT(J,KK,K)                                        RAT00730
      SUM1=SUM1+XRAT(J,KK,K)                                         RAT00740
   10 CONTINUE                                                       RAT00750
      IF(SUM)35,34,35                                                RAT00760
   35 AVG(J,KK) = SUM/XN                                             RAT00770
   34 IF(SUM1) 36,20,36                                              RAT00780
   36 XAVG(J,KK) = SUM1/XNN                                          RAT00790
   20 CONTINUE                                                       RAT00800
   30 CONTINUE                                                       RAT00810
      WRITE(6,102) (EL(I),EL(KK),KK=1,KSTOP)                         RAT00820
      IF(KSTOP-2)47,47,46                                            RAT00830
   47 KLJ=2                                                          RAT00840
      NN=0                                                           RAT00850
      GO TO 45                                                       RAT00860
   46 KLJ=1                                                          RAT00870
      NN=1                                                           RAT00880
   45 DO 50 J=1,NEXP,KLJ                                             RAT00890
      LJ=J+1                                                         RAT00900
      WRITE(6,104)                                                   RAT00910
      DO 51 JJ=1,7                                                   RAT00920
      WRITE(6,100) J,JJ,(RAT(J,KK,JJ),XRAT(J,KK,JJ),MIS(J,KK,JJ),KK=1, RAT00930
     XKSTOP)                                                         RAT00940
      IF(NN)51,53,51                                                 RAT00950
   53 WRITE(6,107) LJ,JJ,(RAT(LJ,KK,JJ),XRAT(LJ,KK,JJ),MIS(LJ,KK,JJ),KK RAT00960
     X=1,KSTOP)                                                      RAT00970
   51 CONTINUE                                                       RAT00980
      WRITE(6,103) (AVG(J,KK),XAVG(J,KK),KK=1,KSTOP)                 RAT00990
      IF(NN)50,48,50                                                 RAT01000
   48 WRITE(6,108) (AVG(LJ,KK),XAVG(LJ,KK),KK=1,KSTOP)               RAT01010
   50 CONTINUE                                                       RAT01020
   40 CONTINUE                                                       RAT01030
C                                                                    RAT01040
C     FORMAT STATEMENTS                                              RAT01050
C                                                                    RAT01060
   98 FORMAT(1H1)                                                    RAT01070
   99 FORMAT(1H2,57X,16HINTENSITY RATIOS  //,37X,59H THE FOLLOWING ELEMERAT09300
     XNTS ARE CONSIDERED INTERNAL STANDARDS-    ,//,46X,(4(A6,4X)))  RAT09350
  100 FORMAT(1H ,2I4,4X,(4(2G11.4,A3)))                              RAT09380
  101 FORMAT(1H0,15X,105H COLUMNS 1,4,7,10 ARE BACKGROUND CORRECTED RATIRAT01110
     XOS.  COLS. 2,5,8,11 ARE THE UNCORRECTED RATIOS.          )     RAT01120
  102 FORMAT(1H1,12H EXP  STEP  ,X,4(A6,2H /,A6,11X))                RAT09500
  103 FORMAT(1H ,5X,3HAVG,4X,(4(2G11.4,3X)) )                        RAT01140
  104 FORMAT (1H0)                                                   RAT01150
  105 FORMAT(1H0,35X,60H * IN COL. 3,6,9,12 MEANS VALUE OF STD. IS EXTRARAT01160
     XPOLATED.        )                                              RAT01170
  106 FORMAT(1H0,32X,64H A BLANK IN THESE COLUMNS MEANS RATIO  WAS CALCURAT01180
     XLATED DIRECTLY.                    )                           RAT01190
  107 FORMAT(1H+60X,2I4,(2(2G11.4,A3))       )                       RAT01200
  108 FORMAT(1H+64X,3HAVG,2X,(2(2G11.4,3X)) )
      RETURN                                                         RAT01220
      END                                                            RAT01230
```

APPENDIX C

SAMPLE OUTPUT FROM SUBROUTINE RATIO

The following output is a typical example from the subroutine RATIO:

INTENSITY RATIOS

THE FOLLOWING ELEMENTS ARE CONSIDERED INTERNAL STANDARDS-

A 4044   W 4008   AG2929   AG3501

COLUMNS 1,4,7,10 ARE BACKGROUND CORRECTED RATIOS. COLS. 2,5,8,11 ARE THE UNCORRECTED RATIOS.

* IN COL. 3,6,9,12 MEANS VALUE OF STD. IS EXTRAPOLATED.

A BLANK IN THESE COLUMNS MEANS RATIO WAS CALCULATED DIRECTLY.

EXP	STEP	NI3566 /A 4044			NI3566 /W 4008			NI3566 /AG2929			NI3566 /AG3501		
1	1	0.1459	0.1743	*	32.655	5.0638		0.3581	0.4277		0.1020	0.1218	*
1	2	0	0		0	0		0	0		0	0	
1	3	0	0		0	0		0	0		0	0	
1	4	0	0		0	0		0	0		0	0	
1	5	0	0		0	0		0	0		0	0	
1	6	0	0		0	0		0	0		0	0	
1	7	0	0		0	0		0	0		0	0	
	AVG	0.1459	0.1743		32.655	5.0638		0.3581	0.4277		0.1020	0.1218	
2	1	0	0		0	0		0	0		0	0	
2	2	0	0.8380	*	0	0.8663E-01	*	0	0.2285	*	0	0.1537	*
2	3	0	0.8498		0	0.8785E-01	*	0	0.2317	*	0	0.1558	*
2	4	0	0.9295		0	0.8646E-01	*	0	0.2281	*	0	0.1534	*
2	5	0	0		0	0		0	0		0	0	
2	6	0	0		0	0		0	0		0	0	
2	7	0	0		0	0		0	0		0	0	
	AVG	0	0.8724		0	0.8698E-01		0	0.2294		0	0.1543	
3	1	0	0		0	0		0	0		0	0	
3	2	0	0		0	0		0	0		0	0	
3	3	0	0		0	0		0	0		0	0	
3	4	0	2.9449	*	0	0.1648	*	0	0.8834		0	0.6593	
3	5	0	3.1737	*	0	0.1776	*	0	0.9145		0	0.7719	
3	6	0	0		0	0		0	0		0	0	
3	7	0	0		0	0		0	0		0	0	
	AVG	0	3.0593		0	0.1712		0	0.8990		0	0.7156	
4	1	0.2297	0.2774	*	0.3154E-01	0.3810E-01	*	0.6918E-01	0.8356E-01	*	0.5894E-01	0.7119E-01	*
4	2	0.2630	0.2818		0.3611E-01	0.3870E-01	*	0.7920E-01	0.8488E-01	*	0.6748E-01	0.7231E-01	*
4	3	0	0		0	0		0	0		0	0	
4	4	0	0		0	0		0	0		0	0	
4	5	0	0		0	0		0	0		0	0	
4	6	0	0		0	0		0	0		0	0	
4	7	0	0		0	0		0	0		0	0	
	AVG	0.2463	0.2796		0.3383E-01	0.3840E-01		0.7419E-01	0.8422E-01		0.6321E-01	0.7175E-01	

5	1	0.9671E-01	0.1359	*	0.7482E-02	0.1052E-01	*	0.4045E-01	0.5685E-01	*	0.3139E-01	0.4412E-01	*
5	2	0.1244	0.1379		0.9628E-02	0.1067E-01	*	0.5206E-01	0.5769E-01	*	0.4040E-01	0.4477E-01	*
5	3	0	0		0	0		0	0		0	0	
5	4	0	0		0	0		0	0		0	0	
5	5	0	0		0	0		0	0		0	0	
5	6	0	0		0	0		0	0		0	0	
5	7	0	0		0	0		0	0		0	0	
	AVG	0.1106	0.1369		0.8555E-02	0.1059E-01		0.4625E-01	0.5727E-01		0.3590E-01	0.4445E-01	
6	1	0	0		0	0		0	0		0	0	
6	2	0	0		0	0		0	0		0	0	
6	3	0	0		0	0		0	0		0	0	
6	4	0	4.9703	*	0	0.7166	*	0	0.9195		0	0.6623	
6	5	0	5.0939	*	0	0.7344		0	0.8736		0	0.7682	
6	6	0	0		0	0		0	0		0	0	
6	7	0	0		0	0		0	0		0	0	
	AVG	0	5.0321		0	0.7255		0	0.8965		0	0.7153	
7	1	0	0		0	0		0	0		0	0	
7	2	0	0.8036		0	0.1225	*	0	0.2686	*	0	0.2009	*
7	3	0	1.0517		0	0.1363	*	0	0.2988	*	0	0.2235	*
7	4	0	0		0	0		0	0		0	0	
7	5	0	0		0	0		0	0		0	0	
7	6	0	0		0	0		0	0		0	0	
7	7	0	0		0	0		0	0		0	0	
	AVG	0	0.9276		0	0.1294		0	0.2837		0	0.2122	
8	1	0	0.4080	*	0	0.9922E-01	*	0	0.1167	*	0	0.9206E-01	*
8	2	0	0.4189	*	0	0.1019	*	0	0.1199	*	0	0.9452E-01	*
8	3	0	0		0	0		0	0		0	0	
8	4	0	0		0	0		0	0		0	0	
8	5	0	0		0	0		0	0		0	0	
8	6	0	0		0	0		0	0		0	0	
8	7	0	0		0	0		0	0		0	0	
	AVG	0	0.4135		0	0.1005		0	0.1183		0	0.9329E-01	

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